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INFERRING NETWORK CONTROLS FROM TOPOLOGY USING THE CHOMP DATABASE

John Harer
DUKE UNIVERSITY

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Final Report

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Final Report

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November 30, 2015

1 John Harer Research

In order to analyze networks dynamically, we developed a variety of tools for applying and computing Topological Data Analysis invariants.

1.1 SW1PerS

A significant development during the project was the development of a theoretical framework and applications for the topological study of time series data [21]. Broadly speaking, we have studied the geometrical and topological properties of sliding window embeddings, as seen through the lens of persistent homology. In particular, we have shown that maximum persistence at the point-cloud level can be used to quantify periodicity at the signal level, proven structural and convergence theorems for the resulting persistence diagrams, and derived estimates for their dependency on window size and embedding dimension. We have also applied this methodology to quantifying periodicity in synthetic data sets, and compared the results with those obtained using state-of-the-art methods in gene expression analysis. We call this new method SW1PerS, which stands for Sliding Windows and 1-dimensional Persistence Scoring. More recently we have used SW1PerS to study physiological data and to look for common patterns in signals. This latter task is a major effort in all of our work for the Air Force as we see it as a revolutionary way to study hidden patterns and discover interesting structure for multi-INT data.

1.2 Frechet Means of Persistence Diagrams

In order to use persistence diagrams as a true statistical tool, it is very useful to have a good notion of mean and variance for a set of diagrams. On this project Harer and collaborators Mileyko, Turner, Mukherjee, Bendich, Mattingly and Munch showed that such a mean and variance exist and developed algorithms to compute them [17], [24]. This work was also extended this work by altering the original definition of Frechet mean so that it now becomes a probability measure on the set of persistence diagrams; in a nutshell, the mean of a set of diagrams is a weighted sum of atomic measures, where each atom is itself the Frechet mean persistence diagram of a perturbation of the input diagrams [19]. We showed that this new definition defines a Holder continuous map from the product k copies of D , the persistence diagram space to the space of probability measures on D , and that it is an extremely statistic on vineyards.

1.3 Cover Trees for Fast Computation of Persistence

The theory of cover trees can be applied to a dataset to construct approximations for algorithms such as k nearest neighbors. Sheehy showed that these can also be used to give approximations to the Rips complex for a dataset with the result that the number of simplices that have to be considered is linear in the number of points [22]. In addition, Kerber and others now have fast algorithms for reducing a persistence matrix: <https://code.google.com/p/phat/>. Combined with a fast algorithm for finding cliques in a graph, this **almost** gives a very fast method for computing persistence. What is missing is the construction of the matrix to reduce. We developed a fast algorithm for doing this, based on a sophisticated hashing algorithm.

1.4 Tracking

We also applied persistence to the analysis of tracking information based on activity of agents under surveillance.

2 Konstantin Mischaikow Research

Given an explicit continuous dynamical system generated by a nonlinear map or differential equation the robust dynamics can be extracted with mathematical rigor via a *finite* set of computations. There are four essential steps to this procedure: (i) discretization of phase space via a grid, (ii) construction of a multivalued map or directed graph defined on the grid that provides an outer approximation of the dynamics of interest, (iii) graph algorithms to decompose the dynamics, and (iv) computation of algebraic topological invariants such as the Conley index using the directed graph information. Each of these steps has a well defined relation to the original dynamics. The choice of grid in step (i) determines the resolution at which the variables of the dynamical system is measured. The

numerical bounds used to determine the outer approximation in step (ii) provide bounds on the precision of the model used to generate the dynamical system or the size of the noise associated with the dynamical system. There are different approaches to the decompositions in step (iii) and they result in information about the gradient-like or recurrent like structure of the system. Step (iv) is used to provide a mathematical guarantee that the dynamics identified by the numerical computations are in fact true solutions and not numerical artifacts. Recent examples of how these ideas fit together in the context of multiparameter systems can be found in [1, 2]. We have also demonstrated that it is possible to use these ideas to efficiently compute mathematically rigorous global Lyapunov functions for nonlinear systems using these methods [5].

We are working on extending these ideas and techniques to the setting of time series data.

2.1 Homology computations

Using ideas from discrete Morse theory we have developed a preprocessing technique that in practice greatly reduces the size of the complexes on which the computation of homology has to be performed. We use this technique to compute the induced map on homology as follows. Given an outer approximation with acyclic values of a continuous function, the projection map from the graph of the multivalued map to the domain of the function induces an isomorphism on homology. Using the Morse preprocessing one computes generators of homology on the domain and the range. The induced map on homology is then obtain by composing on the level of homology the inverse of the projection on the domain with the projection on the range. The advantage of this approach is that the size of the complexes in both the domain and the range is greatly reduced. This work has been published [8] and open source code is provided [6].

The efficiency of the Morse preprocessing is based on reducing the original complex to a much smaller complex. Simple experiments with the code indicate that for complicated higher dimensional complexes the resulting complex depends on the order in which the cells of the original complex are processed. What is clear from our experimental work is that on average we obtain optimal results by alternating the reduction process using collapse and co-collapse operations. We are preparing a paper that explains this procedure and discusses the experimental results [16].

With V. Nanda, a former Ph.D. student, we have used the above mentioned discrete Morse theory methods to develop an efficient preprocessing algorithm to reduce the number of cells in a filtered cell complex while preserving the homology of the filtration, this implies in particular that the persistent homology of the reduced filtration matches the persistent homology of the original filtration. We have successfully applied this technique to the experimental and numerical data in the context of dense granular media. This work has been published [18] and open source code is provided [20].

In the context of time series data or computation of outer approximations using non-convex images we can obtain non-acyclic valued cellular maps. Thus the above mentioned algorithms do not directly apply. The information at our disposal is the graph of the multivalued map $\Gamma \subset X \times X$, the projection map $p: \Gamma \rightarrow X$ onto the domain and the projection map $q: \Gamma \rightarrow X$ to the range. The lack of acyclicity implies that we cannot assume $p_*: H_*(\Gamma) \rightarrow H_*(X)$ is invertible, thus the minimal well defined information that can be extracted is $G_*: \text{image } p_* \rightarrow \frac{H_*(X)}{q_* \ker p_*}$. We are actively exploring the structure of this map under hypothesis relevant to time series data and what information is contained in this map under these conditions. A paper detailing results has been accepted for publication [7].

2.2 Computational Theory for the Decomposition of Nonlinear Dynamics

The classical theory of dynamical systems is based on the existence and structure of invariant sets. However, since each orbit is an invariant set, most physically interesting nonlinear dynamical systems contain uncountably many invariant sets. Chaotic dynamics and bifurcation theory developed over the last 50 years shows that there is no natural countable set of invariant sets that one can restrict one attention to describe global nonlinear dynamics. Thus, on a fundamental level the classical formulation of nonlinear dynamic means that it is not computable.

We are developing an alternative framework for nonlinear dynamics that is explicitly based on grids and outer approximations which at any give level of resolution are countable. We are in the process of comparing the computable structures in our novel approach to dynamics with the classical notions of Morse decompositions and isolated invariant sets. A paper demonstrating that there are no fundamental obstacles to computing Morse decompositions [9] has appear and a paper demonstrating that convergence to classical structures is obtained by refining the approximation methods, i.e. the grids and the outer approximations has been accepted [10]. Another paper explicitly relating the structure of the lattice of attractors to Morse decompositions is in preparation [11].

2.3 Constructing Multivalued Cellular Maps from Time Series Data

Given a time series generated by a continuous map from a manifold to itself we construct associated Cech complexes and a simplicial map between the complexes. Extending the ideas of P. Nyogi, S. Smale, and S. Weinberger to obtain a lower bound on the probability that a continuous selector of the simplicial map corresponds to the same homotopy type of the original map. In particular, this gives us a lower bound on the induced map on homology. This work has been published [3].

2.4 Analysis of Time Series Data of Persistence Diagrams

We are focussing on the analysis of time series data arising from spatio-temporally complex systems arising from fluid dynamics, dense granular material, and social networks. We remark that for each of these systems *each* time point is a high dimensional data set. We reduce the information at each time point by computing a persistence diagram that captures the essential geometric information. Thus our time series consists of a series of points in the space of persistence diagrams. By studying the dynamics in the space of persistence diagrams we are revealing features about otherwise extremely high dimensional systems. We are actively pursuing different methods for using metrics such as bottleneck and Wasserstein on these point clouds of persistence diagrams to characterize the underlying dynamics. The efficiency of the code [20] is critical for these applications since we literally need to be able to compute millions of persistence diagrams.

We have applied these techniques to the study of molecular dynamics simulations of systems of dense granular media under compression. A paper showing that these techniques distinguish the force network structures of particles of dense granular media according to their frictional properties and the polydispersity of the particles has been published [12]. We have also published a paper that provides a mathematical proof of the stability that this approach to the study of time series of particulate systems [14]. That is we show that small errors in the experimental or numerical protocols lead to small changes in the results reported by our approach. We use these techniques to study the spatial properties of the temporal evolution of these systems [13].

We show that similar ideas are applicable to the analysis of dynamics arising from simulations to convection of fluids [15].

We have applied these techniques to the study of the dynamics on random geometric graphs, i.e. graphs which are dominated by "short" edges that arise from an underlying geometric structure but also have a random "long" edges. We show that for certain ranges noise and the thresholds for propagation of information through the network, these topological methods can be used to recover the structure of the underlying network [23].

Though not in the context of time series data we have successfully applied ideas from persistent homology to the analysis of compressibility of proteins [4].

3 Sayan Mukherjee Research

3.1 Consistency of maximum likelihood estimation for some dynamical systems

In a paper that will appear in the Annals of Statistics the following results were shown:

We consider the asymptotic consistency of maximum likelihood parameter estimation for dynamical systems observed with noise. Under suitable conditions on the dynamical systems and the observations, we show that maximum likelihood parameter estimation is

consistent. Our proof involves ideas from both information theory and dynamical systems. Furthermore, we show how some well-studied properties of dynamical systems imply the general statistical properties related to maximum likelihood estimation. Finally, we exhibit classical families of dynamical systems for which maximum likelihood estimation is consistent. Examples include shifts of finite type with Gibbs measures and Axiom A attractors with SRB measures.

This is the first paper that gives rigorous results for consistency of parameter estimation for deterministic dynamical systems with noise. This extends recent results for hidden Markov models. The challenge is that one needs to use ergodic theory instead of stochastic process theory to prove the results.

The main result of the paper is:

Suppose that we have a parametrized family of dynamical systems on

$(T_\theta, \mu_\theta)_{\theta \in \Theta}$ is a parametrized family of dynamical systems on (X, \mathcal{X}) with corresponding observation densities $(g_\theta)_{\theta \in \Theta}$. If certain conditions hold (these were given in an earlier report, then any approximate MLE is consistent at θ_0 .

3.2 Review Article on Dynamical Systems

We have a paper under review in Statistical Surveys that is a review on inference in dynamical systems:

The topic of statistical inference for dynamical systems has been studied widely across several fields. In this survey we focus on methods related to parameter estimation for nonlinear dynamical systems. Our objective is to place results across distinct disciplines in a common setting and highlight opportunities for further research.

3.3 Sufficient statistics for surfaces and shapes

We have developed methodology, theory, and code to model surfaces and shapes. A paper is currently under review in Information and Inference.

We introduce a statistic, the persistent homology transform (PHT), to model surfaces in \mathbb{R}^3 and shapes in \mathbb{R}^2 . This statistic is a collection of persistence diagrams – multiscale topological summaries used extensively in topological data analysis. We use the PHT to represent shapes and execute operations such as computing distances between shapes or classifying shapes. We prove the map from the space of a simplicial complexes in \mathbb{R}^3 into the space spanned by this statistic is injective. This implies that the statistic is a sufficient statistic for distributions on the space of “smooth” shapes. We also show that a variant of this statistic, the Euler Characteristic Transform (ECT), admits a simple exponential family formulation which is of use in providing likelihood based inference for shapes and surfaces. We illustrate the utility of this statistic on simulated and real data.

We are currently using this method for a variety of applications

1. Quantitative and statistical genetics of shape phenotypes.
2. Regression models of behavioral networks.
3. Evolutionary models of shape spaces and morphology.
4. Graph isomorphism problems.

3.4 Dimension reduction

The following formulation of dimension reduction for dynamical systems is a recent project. Using the following framework we are able to integrate classic ideas from Bayesian time series models such as Dynamic Linear Models (DLMs) with classic ideas in topological dynamics such as Markov partitions. The practical utility of these ideas are we are developing dimension reduction methods for both continuous space dynamical systems as well as discrete state dynamical systems.

Given a dynamical system defined by the following (stochastic) maps

$$f : Z_t \rightarrow Z_{t+1}$$

$$g : Z_t \rightarrow Y_t.$$

We consider the following dimension reduction procedure. We are given stochastic maps $\psi : Z_t \rightarrow W_t$ where W is much lower dimensional than Z and $\phi : W_t \rightarrow Z_t$ as well as the dynamics in the lower dimension $q : W_t \rightarrow W_{t+1}$.

Given the above set of maps we can define the following losses to define the goodness of a dimension reduction method specified by (ψ, ϕ, q) :

- (1) Prediction: $\mathbb{E}[l(Y_t | (Y_0^{t-1}, Z_0^t), Y_t | (Y_0^{t-1}, W_0^t))]$
- (2) Filtering: $D_{KL}(p(Z_0^t | Y_0^t), p(Z_0^t | W_0^t))$.

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Abstract

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Changes in research objectives (if any):

None

Change in AFOSR Program Manager, if any:

Original Manager Robert Bonneau

Current Manager Tristan Nguyen

Extensions granted or milestones slipped, if any:

None

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, \$K)

| | Starting FY | FY+1 | FY+2 |
|----------------------|-------------|------|------|
| Salary | | | |
| Equipment/Facilities | | | |
| Supplies | | | |
| Total | | | |

Report Document

Report Document - Text Analysis

Report Document - Text Analysis

Appendix Documents

2. Thank You

E-mail user

Nov 30, 2015 15:07:30 Success: Email Sent to: john.harer@duke.edu